E vs *k* diagram

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

The parameter k is called the crystal momentum and is a parameter that results from applying Schrödinger wave equation to a single-crystal lattice.

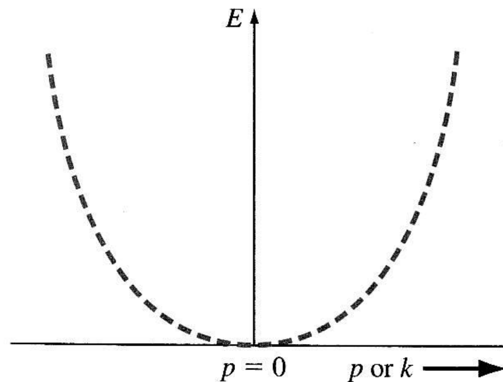


Figure 2.16 | The parabolic E versus k curve for a free electron.

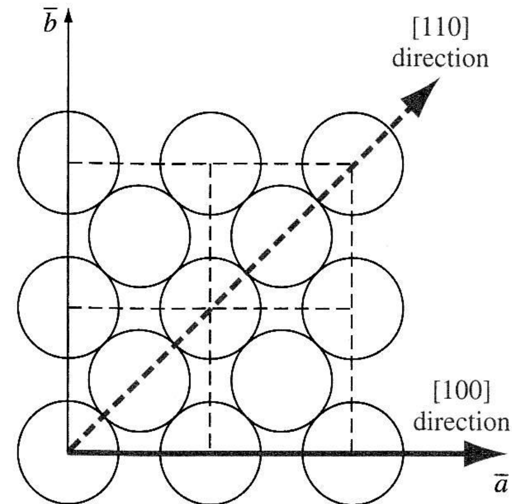


Figure 2.17 | The (100) plane of a face-centered cubic crystal showing the [100] and [110] directions.

Electrons traveling in different directions encounter different potential patterns and therefore different *k*-space boundaries. **The E vs *k* diagrams are in general a function of the *k*-space direction in a crystal**.

Effective mass of carriers – **electrons**

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \longrightarrow m^* = \frac{\hbar^2}{d^2E/dk^2}$$

The effective mass of an electron in a band with a given (E, **k**) relationship

$$E(k) = E_C + \frac{\hbar^2 k^2}{2m_e^*}$$

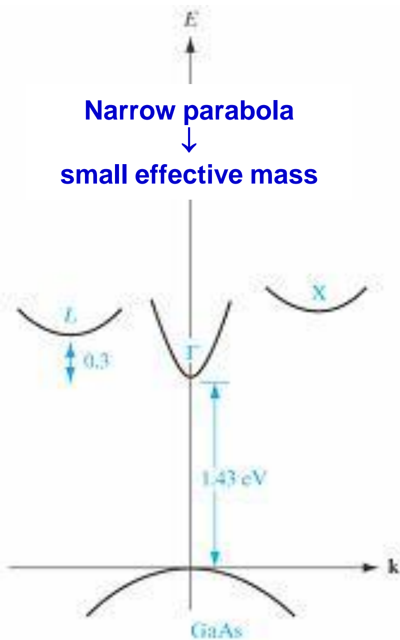
When the conduction band edge occurs at $k = 0$, we can represent the band-structure as a simple parabola,

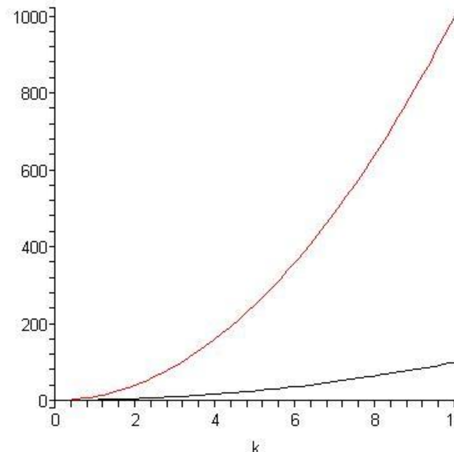
$$m_e^* = \left[\frac{1}{\hbar^2} \cdot \frac{d^2E}{dk^2}\right]^{-1}$$

where:

E_C = minimum of the conduction band energy

m_e* = ***effective mass of an electron***,





GaAs	$m_e^* = 0.063m_0$
Ge	$m_e^* = 0.55m_0$
Si	$m_e^* = 1.09m_0$

Effective mass of carriers – **holes**

Similarly, the energy momentum relation for the valence band can be written…

$$E = E_V - \frac{\hbar^2 k^2}{2m_h^*}$$

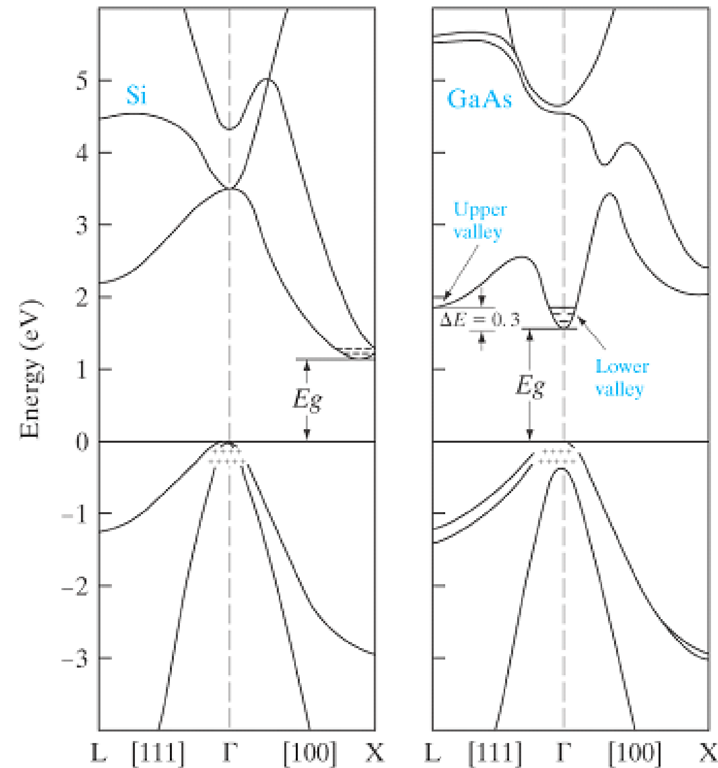
where:

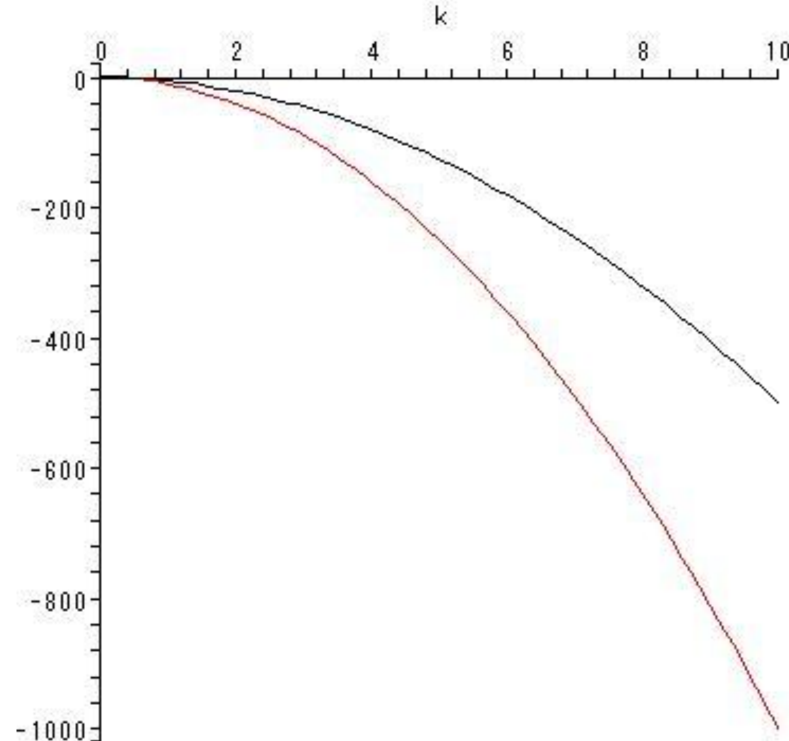
E_V = maximum of the valence band energy

m_h^* = ***effective mass of a hole.***

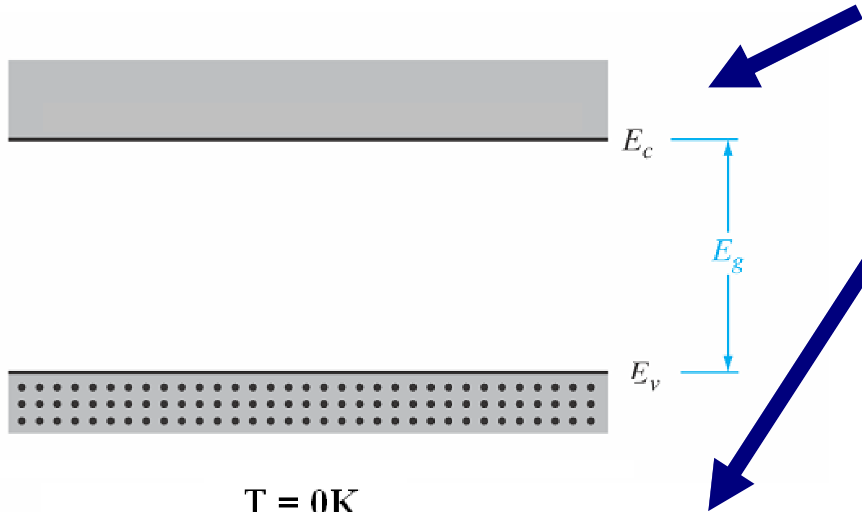
There are actually two bands near the top of the valence band of different widths, leading to ***heavy holes and light holes.***

GaAs	$m_{hh}^* = 0.45m_0$	$m_{lh}^* = 0.08m_0$
Si	$m_{hh}^* = 0.49m_0$	$m_{lh}^* = 0.16m_0$





Intrinsic material



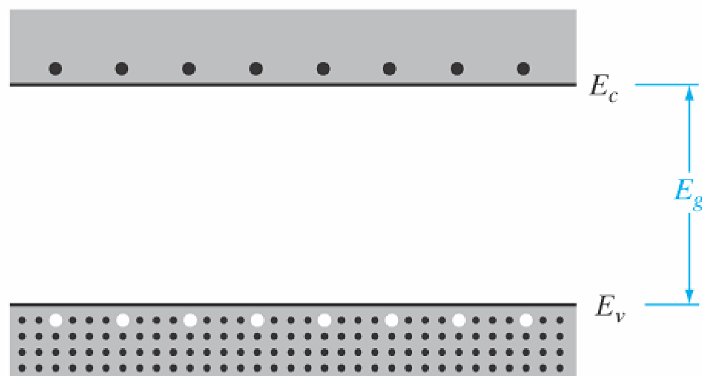


Figure 3.7

Electron–hole pairs in a semiconductor.

- A perfect semiconductor crystal with no impurities or lattice defects is called an intrinsic semiconductor. In such material there are no charge carriers at T = 0 K.
- At higher temperatures EHPs are generated as valence band electrons are thermally excited across the bandgap to the conduction band.
- If a steady state carrier concentration is maintained, there must be recombination of EHPs at the same rate at which they are generated $r_i = g_i$

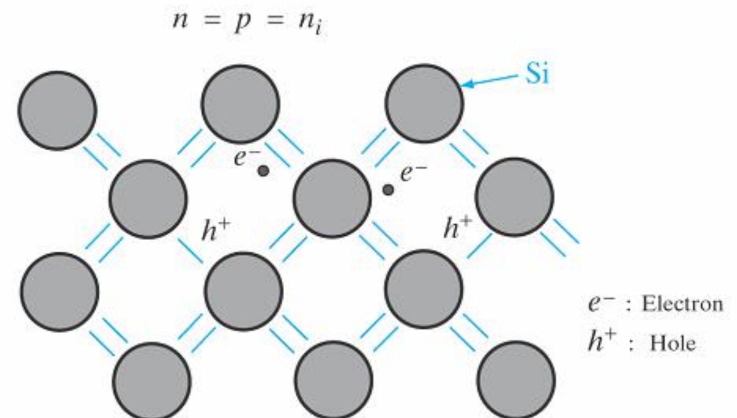


Figure 3.11

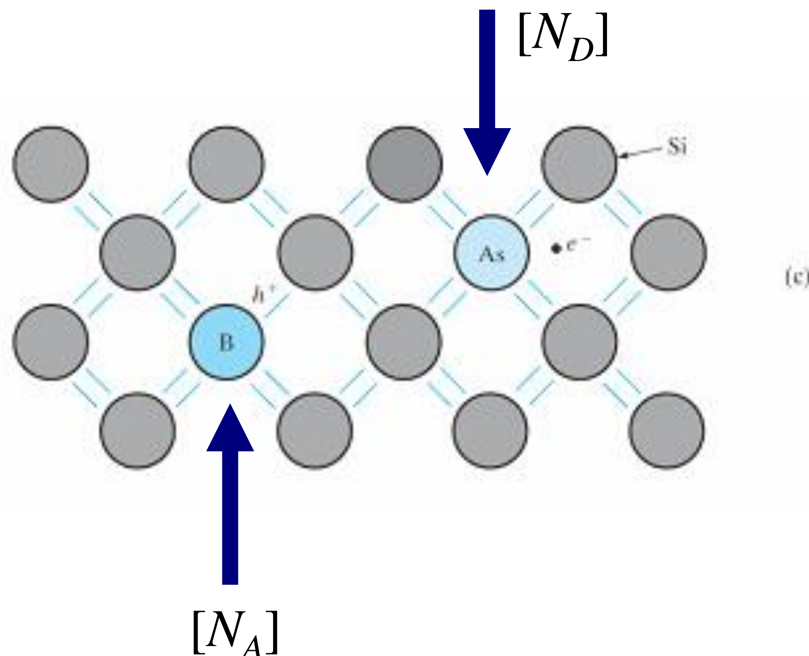
Electron–hole pairs in the covalent bonding model of the Si crystal.

Extrinsic material

In addition to the intrinsic carriers generated thermally … When a group V or III atom (As, B) is substituted into the Si lattice an electron is *donated* or *accepted* and the semiconductor becomes *n*-type or *p*-type respectively.

The crystal is extrinsic when the doping is such that:

$(n_0, p_0) \neq n_i$



In an extrinsic semiconductor at any temperature the carriers concentration have two contributions:

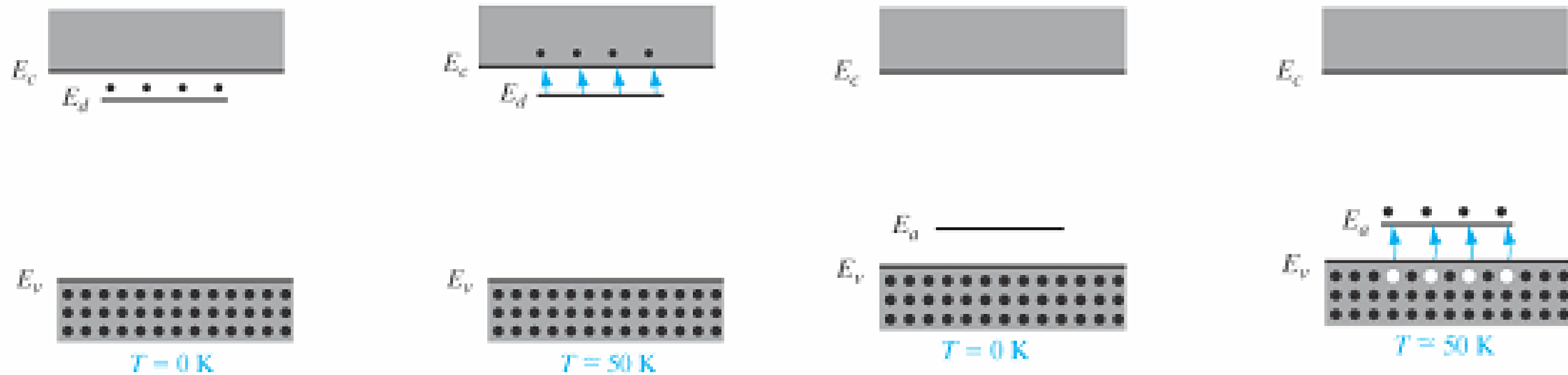
1. Thermal
2. Doping [N_D or N_A]

For a n-type semiconductor:

$$n = N_D \quad \text{and} \quad p = n_i^2 / N_D$$

For a p-type semiconductor:

$$p = N_A \quad \text{and} \quad n = n_i^2 / N_A$$



At 0K the extra electrons associated with the donor atoms are 'fixed' to the donor sites at an energy level E_d.

As the temperature increases there is enough thermal energy to ionize the donor atoms i.e. for an electron to make the transition into the conduction band which is only an energy jump of E_d where $E_d << E_g$.

To create holes in the valence band in a p-type semiconductor, electrons need only an energy of *Ea* to reach the acceptor level where $E_a << E_g$.

Ionization level of dopants

Approximate energy required to excite the 5th electron of a donor atom into the conduction band:

$$E_D = \left(\frac{\varepsilon_0}{\varepsilon_S}\right)^2 \left(\frac{m_e^*}{m_0}\right) E_H$$

→ hydrogen energy levels ⇒ Bohr Model

25 meV for Si
7 meV for GaAs
} donor levels

50 meV for Si, GaAs
V_t= $k_B T/q$ at 300 K = 26 meV
} acceptor levels

In reality, different dopants have different ionization levels and deep levels ($|E| > 3k_BT$), which can be important, but this simple model gives the correct order of magnitude.

Ionization level of dopants

$$E_D = \left(\frac{\varepsilon_0}{\varepsilon_S}\right)^2 \left(\frac{m_e^*}{m_0}\right) E_H$$

Electrons and holes in Quantum Wells

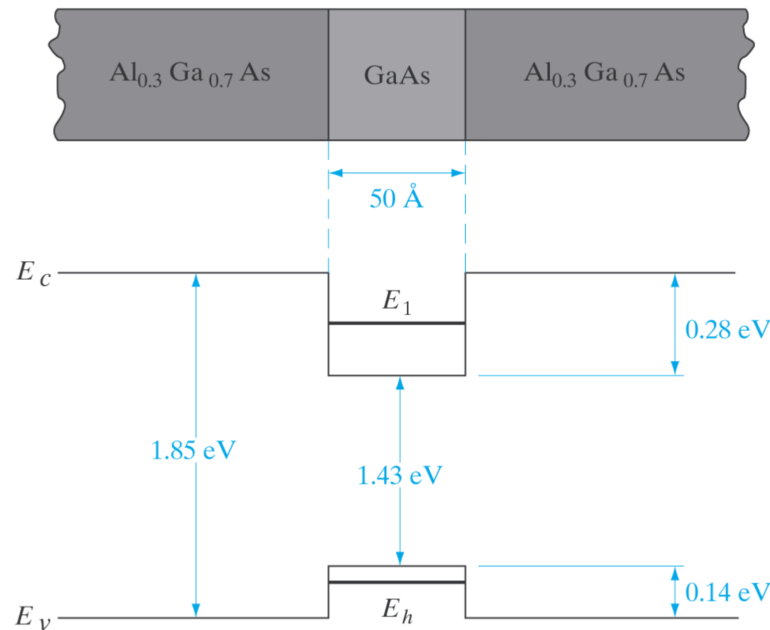


Figure 3.13

Energy band discontinuities for a thin layer of GaAs sandwiched between layers of wider band gap AlGaAs. In this case, the GaAs region is so thin that quantum states are formed in the valence and conduction bands. Electrons in the GaAs conduction band reside on "particle in a potential well" states such as E_1 shown here, rather than in the usual conduction band states. Holes in the quantum well occupy similar discrete states, such as E_h.

A quantum well laser (QWL) is a laser diode in which the active region of the device is so narrow that **quantum confinement** occurs. The wavelength of the light emitted by a QWL is determined by the width of the active region rather than just the bandgap of the material from which it is constructed. This means that much shorter wavelengths can be obtained from QLW than from conventional laser diodes using a particular semiconductor material. The efficiency of a QLW is also greater than a conventional laser diode due to the stepwise form of its **density of states function**.

Density of states function

To obtain the **carrier density per unit volume** we must first calculate the number of allowed states (including spin) per energy range per unit volume.

For electrons in the conduction band where the E-k relation is of the form,

$$E = E_C + \frac{\hbar^2 k^2}{2m_e^*}$$

The density of states is given by:

$$N(E) = 4\pi\left(\frac{2m_e^*}{h^2}\right)^{3/2} E^{1/2}$$

Similarly, for holes in the valence band where the E-k relation is of the form,

$$E = E_V - \frac{\hbar^2 k^2}{2m_h^*}$$

The density of states is given by:

$$N(E) = 4\pi\left(\frac{2m_h^*}{h^2}\right)^{3/2} E^{1/2}$$

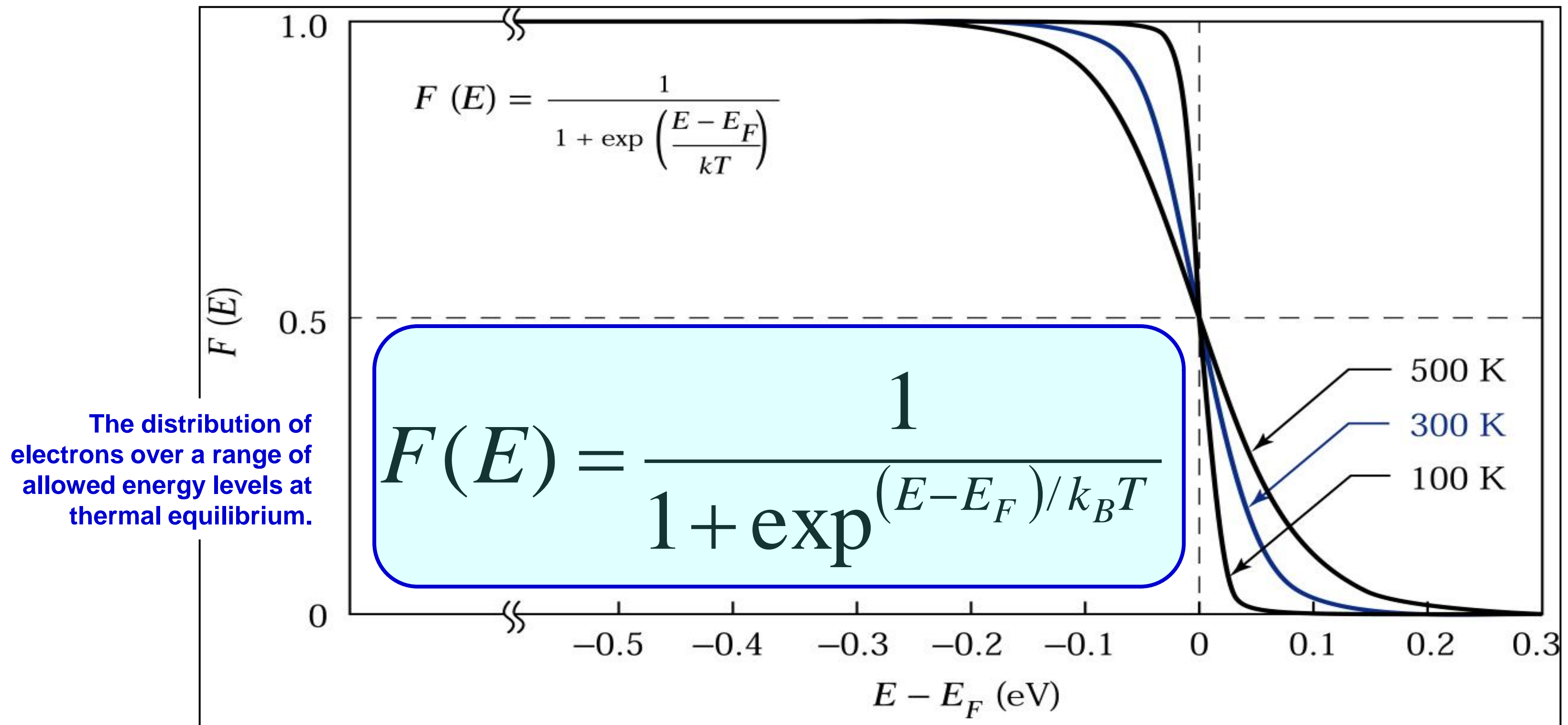
Accounting for the contribution from both *light and heavy holes*

$$m_h^{*\,3/2} = \left(m_{lh}^{*\,3/2} + m_{hh}^{*\,3/2}\right)$$

See appendix IV of Streetman

Fermi-Dirac distribution function

The probability that an electron occupies an electronic state with energy E is given by the ***Fermi-Dirac distribution function***:

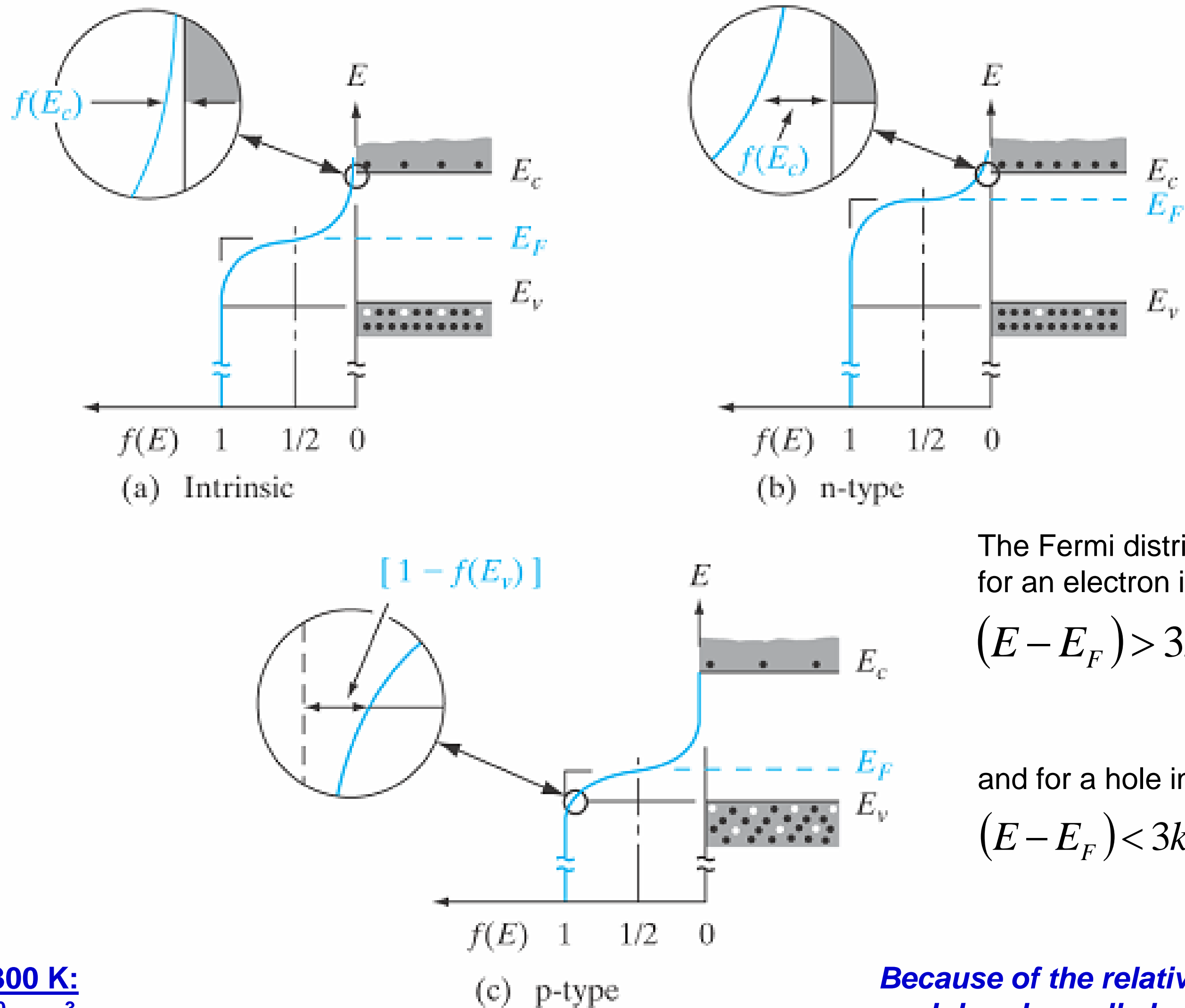


The distribution of electrons over a range of allowed energy levels at thermal equilibrium.

$$F(E) = \frac{1}{1 + \exp^{(E - E_F)/k_B T}}$$

For $E = E_F$ then $F(E) = 0.5$

The Fermi energy is the energy for which the probability of occupation by an electron is exactly ½



The Fermi distribution function is simplified for an electron in the conduction band since,

$$(E - E_F) > 3k_BT \qquad \therefore F(E) \approx e^{-(E-E_F)/k_BT}$$

and for a hole in the valence band since,

$$(E - E_F) < 3k_BT \qquad \therefore F(E) \approx 1 - e^{-(E-E_F)/k_BT}$$

For Si at 300 K:
$n_i = p_i \cong 10^{10}$ cm^{-3}

Density of available states at Ev and Ec:
~ 10^{19} cm^{-3}

Because of the relatively large density of states in each band, small changes in f(E) can result in significant changes in carrier concentration.

Figure 3.15

The Fermi distribution function applied to semiconductors: (a) intrinsic material; (b) n-type material; (c) p-type material.

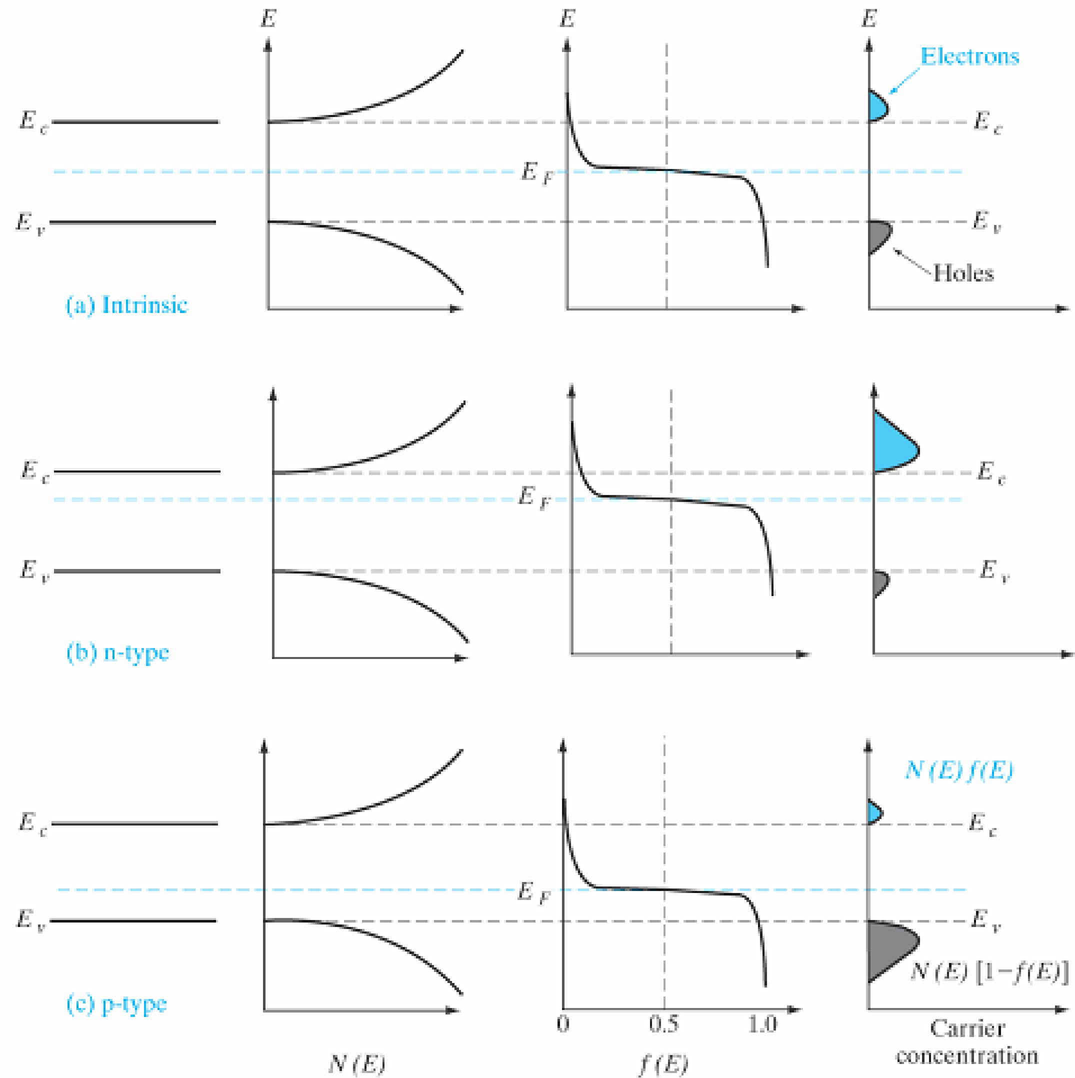
The distribution of electrons in the conduction band is given by the density of allowed quantum states times the probability that a state is occupied by an electron.

The concentration of the electrons in the conduction band is:

$$n = \int_{Ec}^{\infty} f(E)N(E)dE$$

The concentration of the holes in the valence band is:

$$p = \int_{Ec}^{\infty} [1 - f(E)]N(E)dE$$



Electron concentration

The electron density in the conduction band is given by,

$$n = \int_0^{E_{top}\to\infty} n(E)dE = \int_0^{E_{top}\to\infty} N(E)F(E)dE$$

taking the bottom of the conduction band to be E=0

Taking the previous simplified expression for $F(E)$,

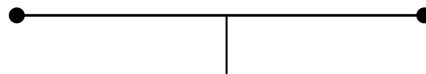
$$n = 4\pi\left(\frac{2m_e^*}{h^2}\right)^{3/2}\int_0^{\infty} E^{1/2}\exp\left(-\frac{E-E_F}{k_B T}\right)dE$$

Electron concentration

Let x = E/kT

$$n = 4\pi\left(\frac{2m_e^*}{h^2}\right)^{3/2}(k_B T)^{3/2}\exp\left(\frac{E_F}{k_B T}\right)\int_0^\infty x^{1/2}e^{-x}dx$$

$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2}\exp\left(\frac{E_F}{k_B T}\right)$$

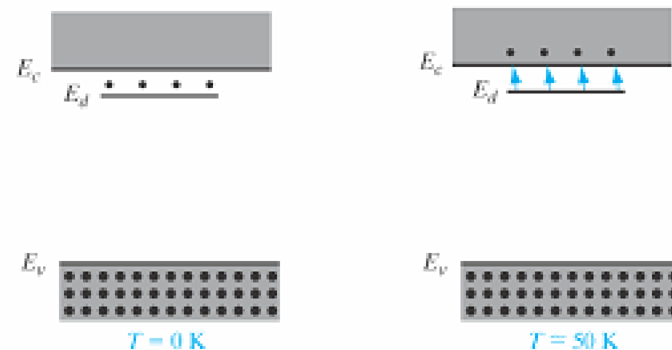


The effective density of states in the conduction band, N_C

Electron concentration

Taking the bottom of the conduction band as E_C rather than E=0,

$$n = N_C \exp\left(-\frac{E_C - E_F}{k_B T}\right)$$



Where:

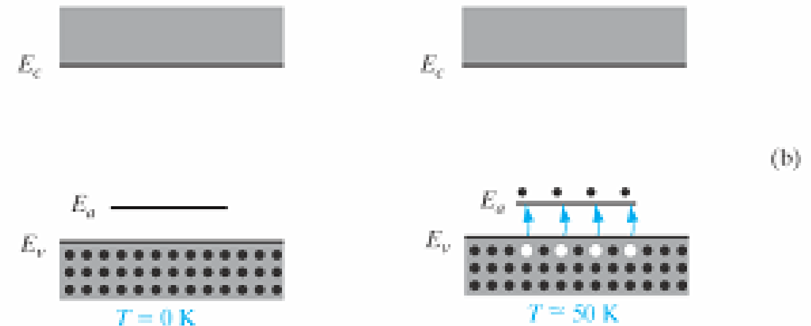
$$Nc = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2}$$

For Si (300 K)	N_C = 2.8 x 10^{19} cm^{-3}
For GaAs (300 K)	N_C = 4.7 x 10^{17} cm^{-3}

Hole concentration

Similarly for holes in the valence band,

$$p = N_V \exp\left(-\frac{E_F - E_V}{k_B T}\right)$$



Where: $$Nv = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2}$$

For Si (300 K)	N_V = 1.04 x 10^{19} cm^{-3}
For GaAs (300 K)	N_V = 7 x 10^{18} cm^{-3}

Law of Mass Action

$$np = n_i^2 = N_C N_V \exp\left(\frac{-E_g}{k_B T}\right)$$

This expression is independent of E_F and is valid for extrinsic (doped) semiconductors too.

$$n_i = \sqrt{N_C N_V} \exp\left(\frac{-E_g}{2k_B T}\right)$$

For Si (300 K)	n_i = 9.65 x 10^9 cm^{-3}
For GaAs (300 K)	n_i = 2.25 x 10^6 cm^{-3}

Law of Mass Action. Intrinsic Semiconductors

$$n = n_i \exp\left(\frac{E_F - E_i}{k_B T}\right) \qquad p = n_i \exp\left(\frac{E_i - E_F}{k_B T}\right)$$

The product *np* is then,

$$np = n_i \exp\left(\frac{E_i - E_F}{k_B T}\right) \bullet n_i \exp\left(\frac{E_F - E_i}{k_B T}\right)$$

$$np = n_i^2$$

So the law of mass action holds also for extrinsic semiconductors.

Calculation of extrinsic Fermi level

At 300 K there is usually enough thermal energy to completely ionize the dopant atoms, so for *n*-type semiconductor $n = N_D$ (donor concentration)

$$n = N_C \exp\left(-\frac{E_C - E_F}{k_B T}\right)$$

$$N_D = N_C \exp\left(-\frac{E_C - E_F}{k_B T}\right)$$

$$\therefore E_C - E_F = k_B T \ln\left(\frac{N_C}{N_D}\right)$$

So as the concentration of <u>donor atoms</u> increases the Fermi level moves closer to the bottom of the conduction band

Calculation of extrinsic Fermi level

Similarly for p-type semiconductors, p = N_A (acceptor concentration)…

$$p = N_V \exp\left(-\frac{E_F - E_V}{k_B T}\right)$$

$$N_A = N_V \exp\left(-\frac{E_F - E_V}{k_B T}\right)$$

$$\therefore E_F - E_V = k_B T \ln\left(\frac{N_V}{N_A}\right)$$

So as the concentration of acceptor atoms increases the Fermi level moves closer to the top of the valence band

Calculation of extrinsic Fermi level

It is often useful to express the carrier density in terms of the intrinsic carrier concentration and the intrinsic Fermi level…

For electrons,

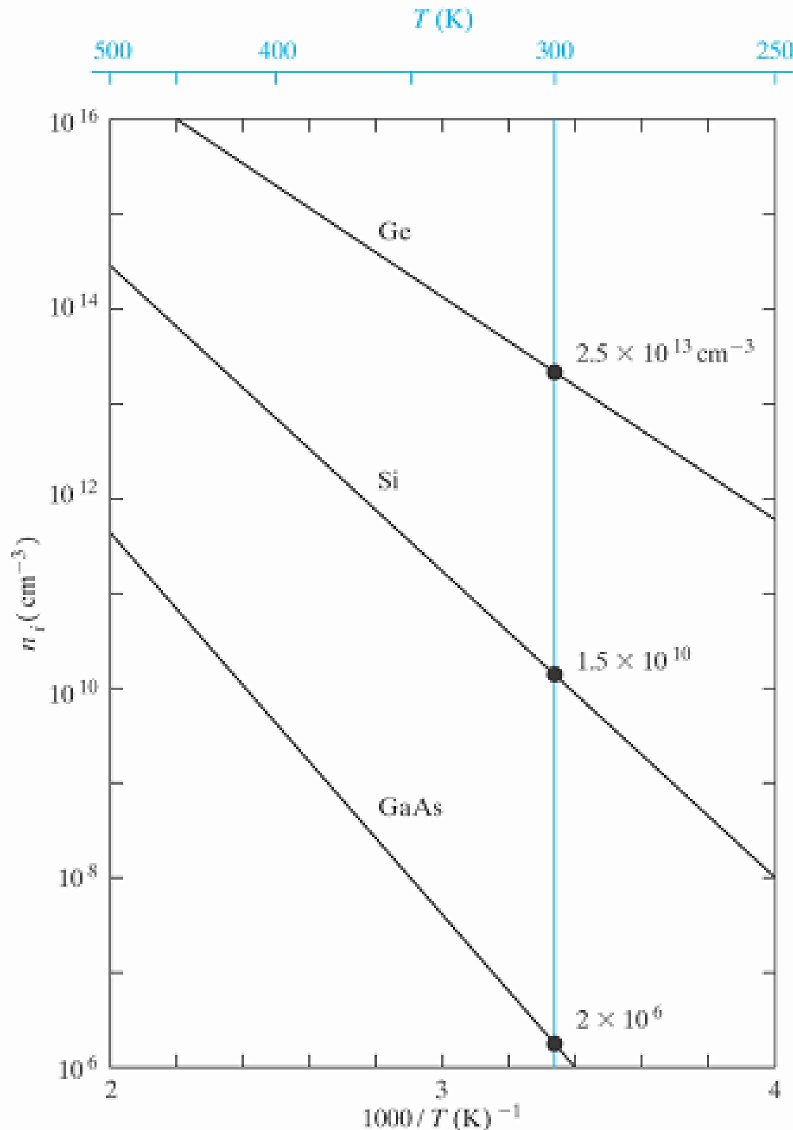
$$n = N_C \exp\left(-\frac{E_C - E_i}{k_B T}\right)\exp\left(-\frac{E_i - E_F}{k_B T}\right)$$

$$n = n_i \exp\left(\frac{E_F - E_i}{k_B T}\right)$$

Similarly for holes,

$$p = n_i \exp\left(\frac{E_i - E_F}{k_B T}\right)$$

Intrinsic carrier densities n_i as a function of temperature



Intrinsic carrier densities in Si, Ge and GaAs as a function of the reciprocal of temperature.

$$n_i = \sqrt{N_C N_V} \exp\left(\frac{-E_g}{2k_B T}\right)$$

E_g (Ge) = 0.66 eV
E_g (Si) = 1.12 eV
E_g (GaAs) = 1.42 eV

For Si (300 K) $n_i = 9.65 \times 10^{9}$ cm^{-3}
For GaAs (300 K) $n_i = 2.25 \times 10^{6}$ cm^{-3}

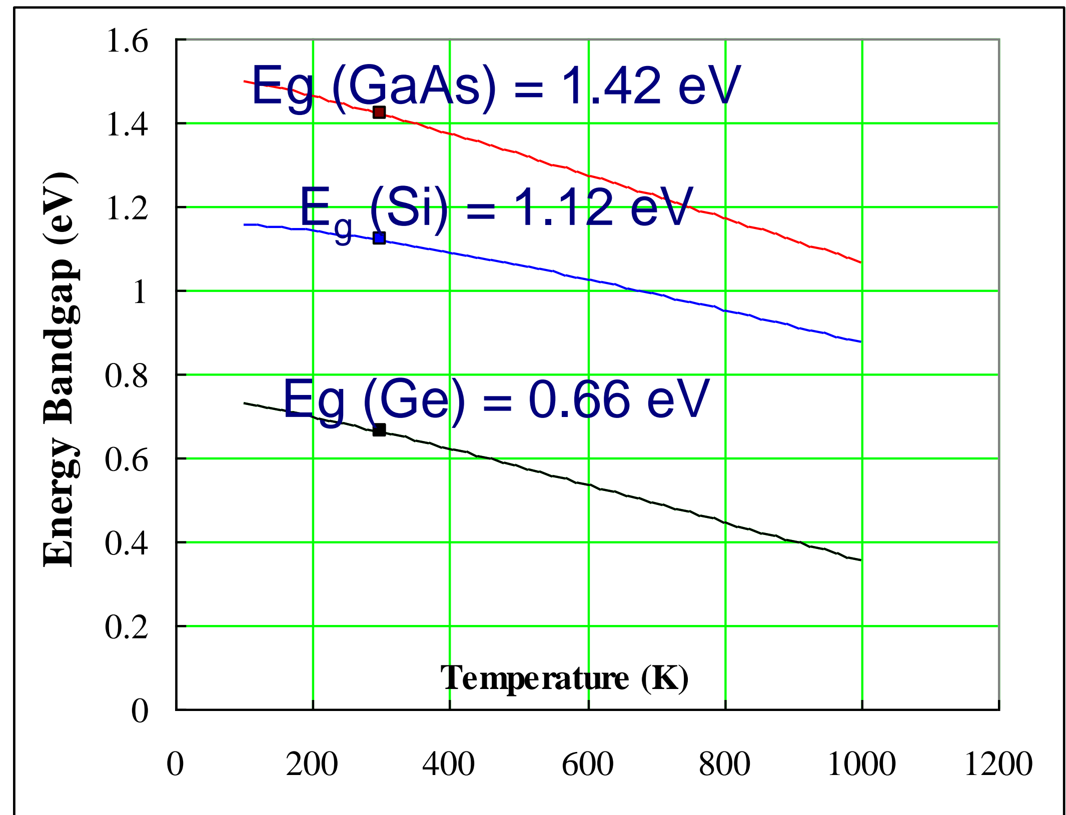
Energy gap E_g as a function of temperature

The temperature dependence of the energy bandgap, E_g, has been experimentally determined yielding the following expression for E_g as a function of the temperature, T:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$

where $E_g(0)$, α and β are the fitting parameters. These fitting parameters are listed for germanium, silicon and gallium arsenide in Table.

	Germanium	Silicon	GaAs
$E_g(0)$ (eV)	0.7437	1.166	1.519
α (meV/K)	0.477	0.473	0.541
β (K)	235	636	204



Electron density n_0 as a function of temperature

At low temperatures the thermal energy is insufficient to ionize all donor atoms so $n < N_D$

At higher temperatures the thermal energy is sufficient to ionize all donor atoms so $n = N_D$

At some temperature the intrinsic carrier density becomes comparable to the donor concentration and beyond this point the semiconductor becomes intrinsic.

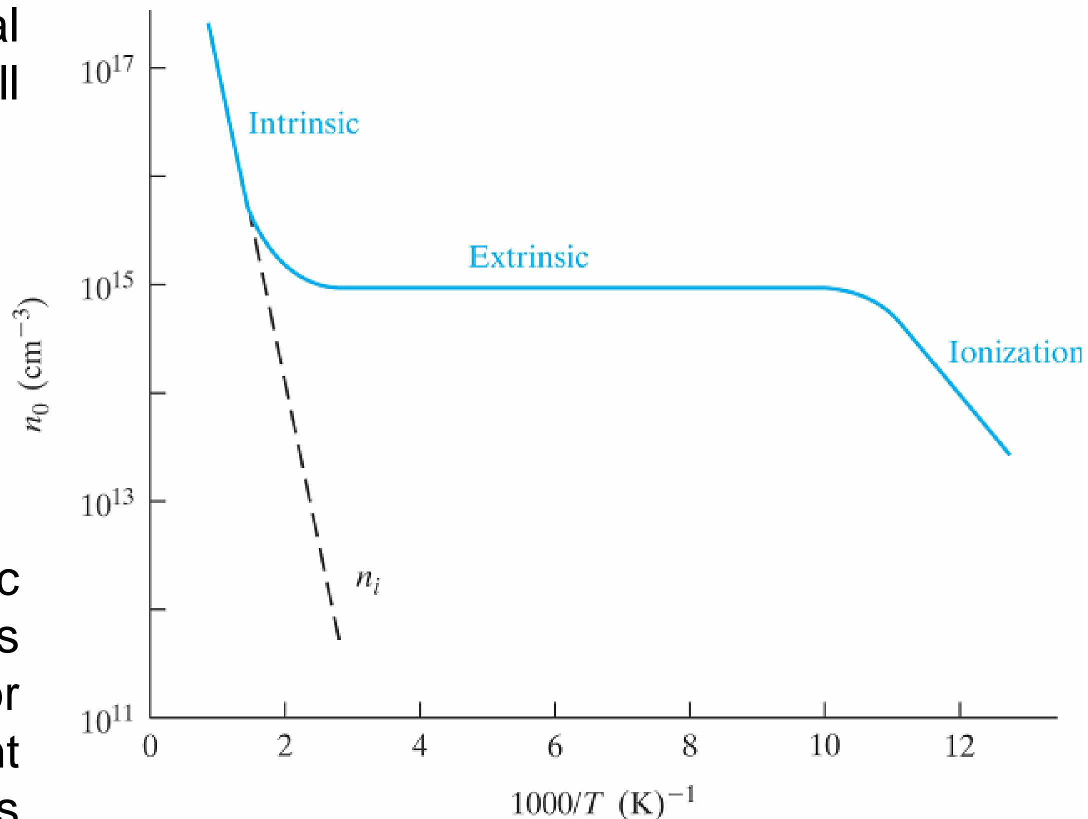


Figure 3.18

Carrier concentration vs. inverse temperature for Si doped with 10^{15} donors/cm^3.